

A toric dynamical system approach to the convergence to equilibrium of quantum Boltzmann equations for Bose gases

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March 1, 2017

Abstract

When the temperature of a trapped Bose gas is below the Bose-Einstein transition temperature and above absolute zero, the gas is composed of two distinct components: the Bose-Einstein condensate and the cloud of thermal excitations. The dynamics of the excitations can be described by quantum Boltzmann models. We prove that the discrete differential equations for these quantum Boltzmann models converge to an equilibrium point. Moreover, this point is unique for all initial conditions that satisfy the same conservation laws. In the proof, we establish a connection between quantum Boltzmann models and chemical reaction networks, and we show that the question about the convergence to equilibrium of quantum kinetic equations is analogous to the global attractor conjecture for chemical reaction networks. We then employ a toric dynamical system approach, similar to the one used to prove the global attractor conjecture, to study the convergence to equilibrium of several types of quantum kinetic equations. Our convergence results also apply to the weak turbulence Boltzmann equation for phonon interactions in anharmonic crystals.

Keywords: quantum Boltzmann equation, weak turbulence, dynamical systems, bosons, Bose-Einstein condensate, excitations-thermal cloud, phonons, quantum theory of solids, rate of convergence to equilibrium, global attractor conjecture, mass-action kinetics, power law systems, biochemical networks, Petri net, Uehling-Uhlenbeck operator, Peierls operator.
MSC: 35Q20, 45A05, 47G10, 82B40, 82B40, 37N25, 92C42, 37C10, 80A30, 92D25.

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1 Introduction

The history of kinetic theory starts with the classical Boltzmann equation, which describes the dynamics of dilute monoatomic gases (cf. [23, 24, 22, 49]). In order to extend the Boltzmann equation from classical particles to quantum particles, the Uehling-Uhlenbeck equation was introduced [71, 84]. However, the Uehling-Uhlenbeck equation is only true for a dilute Bose gas, which is above the Bose-Einstein Condensate (BEC) critical temperature.

After the first observation of the Bose-Einstein condensation of dilute Bose gases in a gas of rubidium ^{87}Rb atoms [5] and then in a gas of sodium ^{23}Na atoms [6], which lead to the 2001 Nobel Prize in physics of Wieman, Cornell and Ketterle [15], there has been a huge amount of research investigating properties of dilute BECs.

Finding a satisfactory theory of symmetry breaking and phase transitions across the BEC critical temperature is an important problem in theoretical physics. In general, the investigation of symmetry breaking and phase transitions is a central to modern physics, and resulted in many Nobel prize awards: Lee-Osheroff-Richardson (1996), Cornell-Ketterle-Weiman (2001). Below the critical temperature, due to many-body effects, the equilibrium distribution depends on quasiparticle energies rather than particle ones [18], which leads to the fact that the $U(1)$ symmetry is broken. As a consequence, a new description in terms of quasiparticles is needed. Such a description should take into account the interatomic interactions which are known to have an important role in the dynamics of the condensing system and should involve both aspects of kinetic theory and quantum mechanics. After the pioneering work of Kirkpatrick and Dorfman [65, 66] deriving a kinetic model for bosonic gases below the BEC critical temperature, there has been an explosion of research on the kinetic theory for BECs (see [80, 29, 79, 59, 65, 66, 88, 81, 51, 82, 11, 12, 1, 86, 62, 63, 67] and references therein). In the series of works [48, 43, 61, 44, 60, 45], Gardinier, Zoller and collaborators introduced the terminology “quantum kinetic theory” and a Master Quantum

Kinetic Equation, which has the Kirkpatrick and Dorfman model as the limit. Notice that it was in Gardiner, Zoller et. al. [48] that the first numerical experiments of condensate growth had been done, before all specific condensate formation data were carried on. These were the first theoretical, quantitative results which have a good agreement with the experiments of [5, 6, 15]. By using the PY method from quantum field theory, Reichl and Gust discovered a new collision operator (cf. [76, 55, 54]). The model of Reichl and Gust is more precise when describing the dynamics of BECs; it can be used to obtain microscopic expressions for the six hydrodynamic modes of a dilute Bose-Einstein condensate: two transverse (shear) modes and four longitudinal modes corresponding to the first sound (density waves) and second sound (temperature waves). We refer to the series of books [74, 46, 83, 47] and the review paper [9] for a complete discussion and more references on this rapidly growing research on quantum gases. We also refer to [78, 77, 68, 52, 16, 13, 30, 69, 17, 36], and cited references, for recent works on the rigorous derivation of nonlinear Schrödinger and related equations starting from the Quantum N-body problem.

Let us recall briefly the main ingredients of the quantum kinetic theory for BECs and excitations: A gas of at temperature T can be considered as quantum-mechanical wavepackets. The thermal de Broglie wavelength, which describes the position uncertainty associated with the thermal momentum distribution, can be computed as $\lambda_{dB} = \left(\frac{2\pi\hbar^2}{mk_B T}\right)^{\frac{1}{2}}$, where m is the mass of the particles and k_B is the Boltzmann constant. When the gas temperature is high $T > T_{BEC}$, the bosons can be regarded as a system of “billiard balls” (cf. [35, 64]). At the BEC transition temperature, λ_{dB} becomes comparable to the distance between bosons and the atomic wavepackets “overlap”. As a result, the indistinguishability of atoms becomes important and the bosons undergo a quantum-mechanical phase transition, which leads to the formation of the BEC (cf. [35, 64]). When the temperature is finite $T_{BEC} > T > 0$ Kelvin, the trapped Bose gas is composed of two distinct components: the high-density condensate, being localized at the center of the trapping potential, and the low-density cloud of thermally excited atoms, spreading over a much wider region (cf. [65, 66, 88]). The dynamics of the thermal cloud atoms is described by quantum Boltzmann models: Equations (1.1) and (1.8).

While the mathematical theory for classical gases has been significantly developed, with the work of Carleman, DiPerna, Lions, Villani and many other mathematicians (for example, see [21, 34, 85, 32, 85]), there are still many open research topics for quantum gases, which need to be explored. An important result on the mathematical side is the work of Escobedo and Velazquez [37], in which they prove that the Uehling-Uhlenbeck equation has a blow-up solution. The aim of our current work is to provide the first mathematical study of the convergence to equilibrium of solutions to the discrete quantum Boltzmann model describing the dynamics of thermal cloud by Kirkpatrick-Dorfman and others, and the modified quantum Boltzmann model by Reichl and Gust.

Quantum Boltzmann model of the thermal cloud.

The quantum Boltzmann equation of the thermal cloud describes the evolution of the density distribution function f of the excited atoms outside of the condensate. The distribution $f(t, p)$ is a function of time t and momenta p . If we denote

$$f_1 = f(t, p_1), f_2 = f(t, p_2), f_3 = f(t, p_3), f_4 = f(t, p_4),$$

then f_1 satisfies

$$\frac{\partial f_1}{\partial t} = C_{12}[f_1] + C_{22}[f_1], \quad (1.1)$$

where

$$C_{22}[f_1] := \int_{\mathbb{R}^9} \mathcal{K}_{p_1, p_2, p_3, p_4}^{22} \delta(p_1 + p_2 - p_3 - p_4) \delta(\mathcal{E}_{p_1} + \mathcal{E}_{p_2} - \mathcal{E}_{p_3} - \mathcal{E}_{p_4}) \quad (1.2)$$

$$\times [(1 + f_1)(1 + f_2)f_3f_4 - f_1f_2(1 + f_3)(1 + f_4)] dp_2 dp_3 dp_4, \quad (1.3)$$

$$C_{12}[f_1] := \int_{\mathbb{R}^6} \mathcal{K}_{p_1, p_2, p_3}^{12} \delta(p_1 - p_2 - p_3) \delta(\mathcal{E}_{p_1} - \mathcal{E}_{p_2} - \mathcal{E}_{p_3}) \quad (1.4)$$

$$\times [(1 + f_1)f_2f_3 - f_1(1 + f_2)(1 + f_3)] dp_2 dp_3 \\ - 2 \int_{\mathbb{R}^6} \mathcal{K}_{p_1, p_2, p_3}^{12} \delta(p_2 - p_1 - p_3) \delta(\mathcal{E}_{p_2} - \mathcal{E}_{p_1} - \mathcal{E}_{p_3}) \\ \times [(1 + f_2)f_1f_3 - f_2(1 + f_1)(1 + f_3)] dp_2 dp_3,$$

and $\mathcal{K}_{p_1, p_2, p_3, p_4}^{22}, \mathcal{K}_{p_1, p_2, p_3}^{12} \geq 0$ are the collision kernels, which are radially symmetric, and symmetric with respect to the permutation of p_1, p_2, p_3 , and p_4 :

$$\mathcal{K}_{p_1, p_2, p_3, p_4}^{22} = \mathcal{K}_{|p_1|, |p_2|, |p_3|, |p_4|}^{22} = \mathcal{K}_{|p_2|, |p_1|, |p_3|, |p_4|}^{22} = \mathcal{K}_{|p_3|, |p_2|, |p_1|, |p_4|}^{22} \\ = \mathcal{K}_{|p_4|, |p_2|, |p_3|, |p_1|}^{22} = \mathcal{K}_{|p_1|, |p_3|, |p_2|, |p_4|}^{22} = \mathcal{K}_{|p_1|, |p_4|, |p_3|, |p_2|}^{22} = \mathcal{K}_{|p_1|, |p_2|, |p_4|, |p_3|}^{22},$$

and

$$\mathcal{K}_{p_1, p_2, p_3}^{12} = \mathcal{K}_{|p_1|, |p_2|, |p_3|}^{12} = \mathcal{K}_{|p_2|, |p_1|, |p_3|}^{12} = \mathcal{K}_{|p_3|, |p_2|, |p_1|}^{12} = \mathcal{K}_{|p_1|, |p_3|, |p_2|}^{12},$$

where $|p|$ denotes the length of the vector p . We suppose that the temperature is very low compared to the Bose-Einstein critical temperature. As a result, the energy $\mathcal{E}_p = \mathcal{E}(p)$ is given by the phonon dispersion law (cf. [75]):

$$\mathcal{E}(p) = c|p|, \quad c = \sqrt{\frac{gn_c}{m}}. \quad (1.5)$$

The operator C_{22} is often referred to as the Uehling-Uhlenbeck collision integral, and describes two-body collisions between excited atoms (2 atoms \rightleftharpoons 2 atoms). The collision operator C_{12} describes collisions which involve one condensate atom (1 atom \rightleftharpoons 2 atoms). Let us note that $\mathcal{K}_{p_1, p_2, p_3}^{12}$ is a function of $n_c, |p_1|, |p_2|, |p_3|$ and it becomes 0 when $n_c = 0$ (cf. [88]).

Nordheim or Uehling-Uhlenbeck equation. If there is no condensate, i.e. $n_c = 0$, then $C_{12} = 0$. As a result, Equation (1.1) can be reduced to the Nordheim or Uehling-Uhlenbeck equation

$$\frac{\partial f_1}{\partial t} = C_{22}[f_1]. \quad (1.6)$$

Quantum Boltzmann equation of phonons and quantum Boltzmann equation of bosons at very low temperature. If the temperature of the quasiparticles in the dilute Bose gas is below the Bose-Einstein transition temperature T_c , one can assume the dominance of the bosons-condensate interactions C_{12} over the bosons-bosons interactions C_{22} and the quantum Boltzmann equation of bosons at very low temperature reads (see [10, 38]):

$$\frac{\partial f_1}{\partial t} = C_{12}[f_1]. \quad (1.7)$$

Interestingly, the quantum *phonon* Boltzmann equation [73, 20] coming from the quantum theory of *solids* has exactly the same mathematical formulation as (1.7). *Moreover, it is in the context of the study of phonon interactions in anharmonic crystals [72] that the first derivation of a kinetic model of weak turbulence was obtained:* R. Peierls suggested the theoretical option of considering the anharmonicities as a small perturbation to the perfectly harmonic crystal, which leads to a kinetic model of an interacting phonons in terms of a nonlinear Boltzmann equation. The phonon Boltzmann equation is then used to carry on the actual computation of the thermal conductivity of dielectric crystals. *Moreover, let us emphasize that in the Zakharov's weak turbulence theory approach to Bose-Einstein condensates, an equation similar to (1.7) has also been obtained (cf. [87]).* As an attempt to build a theory for (1.7), some mathematical results have been obtained in [2, 70, 39].

The modified quantum Boltzmann model of the thermal cloud. As mentioned in the introduction, in [76, 55, 54], Reichl and Gust discovered a new collision operator, which makes the model (1.1)-(1.4) more complicated:

$$\frac{\partial f_1}{\partial t} = C_{12}[f_1] + C_{22}[f_1] + C_{13}[f_1], \quad (1.8)$$

where

$$\begin{aligned} C_{13}[f_1] = & \int_{\mathbb{R}^{3 \times 3}} \mathcal{K}_{p_1, p_2, p_3, p_4}^{13} \delta(p_1 - p_2 - p_3 - p_4) \delta(\mathcal{E}_{p_1} - \mathcal{E}_{p_2} - \mathcal{E}_{p_3} - \mathcal{E}_{p_4}) \\ & \times [(1 + f_1)f_2f_3f_4 - f_1(1 + f_2)(1 + f_3)(1 + f_4)] dp_2 dp_3 dp_4 \\ & - 3 \int_{\mathbb{R}^{3 \times 3}} \mathcal{K}_{p_1, p_2, p_3, p_4}^{13} \delta(p_2 - p_1 - p_3 - p_4) \delta(\mathcal{E}_{p_2} - \mathcal{E}_{p_1} - \mathcal{E}_{p_3} - \mathcal{E}_{p_4}) \\ & \times [(1 + f_2)f_1f_3f_4 - f_2(1 + f_1)(1 + f_3)(1 + f_4)] dp_2 dp_3 dp_4, \end{aligned} \quad (1.9)$$

and C_{12} , C_{22} are defined in (1.3), (1.4) and $\mathcal{K}_{p_1, p_2, p_3, p_4}^{13}$ is positive, radially symmetric, and symmetric with respect to the permutation of p_1, p_2, p_3, p_4

$$\begin{aligned}\mathcal{K}_{p_1, p_2, p_3, p_4}^{13} &= \mathcal{K}_{|p_1|, |p_2|, |p_3|, |p_4|}^{13} = \mathcal{K}_{|p_2|, |p_1|, |p_3|, |p_4|}^{13} = \mathcal{K}_{|p_3|, |p_2|, |p_1|, |p_4|}^{13} \\ &= \mathcal{K}_{|p_4|, |p_2|, |p_3|, |p_1|}^{13} = \mathcal{K}_{|p_1|, |p_3|, |p_2|, |p_4|}^{13} = \mathcal{K}_{|p_1|, |p_4|, |p_3|, |p_2|}^{13} = \mathcal{K}_{|p_1|, |p_2|, |p_4|, |p_3|}^{13}.\end{aligned}$$

Notice that $p = 0$ corresponds to the condensate and it turns out that we need to consider the collisions between atoms only in the high-temperature region with large momenta. Therefore, in this paper, we impose the assumption that $\mathcal{K}_{p_1, p_2, p_3, p_4}^{22}$, $\mathcal{K}_{p_1, p_2, p_3, p_4}^{13}$ become 0 if one of the variables p_1, p_2, p_3, p_4 is 0.

Reaction networks and a toric dynamical system approach for the relaxation to equilibrium problem.

The mathematical program about the trend to equilibrium for kinetic equations was initiated by Desvillettes and Villani in [31, 32]. The study of the relaxation of BECs to thermodynamic equilibrium has also played very important role in the theory of Bose gases [76, 55, 54, 51, 88]. In [39] the authors have proved the existence and uniqueness of solutions of the linearized model of (1.7) satisfying conservation of energy. They have showed that these solutions converge to the corresponding stationary state, at an explicit algebraic rate as time tends to infinity.

Our main tool to study the Peierls model (1.7), the quantum Boltzmann model of the thermal cloud (1.1), and the modified quantum Boltzmann model of the thermal cloud (1.8) is to convert these equations into chemical reaction systems and use an extension of the theory of toric dynamical systems (cf. [26]).

In general, there is great interest in understanding the qualitative behavior of deterministically modeled chemical reaction systems, including the existence of positive equilibria, stability properties of equilibria, and the non-extinction, or persistence, of species, which are the constituents of these systems [41, 42, 57, 3, 7, 50, 14, 4, 26, 33]. Toric dynamical systems – originally called complex-balanced systems (cf. [26, 58]) – are models used to describe an important class of chemical kinetics. The complex-balanced condition was first introduced by Boltzmann [19] for modeling collisions in kinetic gas theory. Based on this condition, it was shown by Horn and Jackson [58, 56, 40, 53] that a complex-balanced system has a unique locally stable equilibrium within each linear invariant subspace. To underline the tight connection to the algebraic study of toric varieties, the name “toric dynamical system” was proposed in [26]. The most important problem in the theory of toric dynamical systems is the Global Attractor Conjecture, which says that the complex balanced equilibrium of a toric dynamical system is a globally attracting point within each linear invariant subspace. This global attractor question is strongly related to the convergence to equilibrium problem in the study of kinetic equations. A proof to the Global Attractor Conjecture for small dimensional systems has been supplied in [28], and a complete proof has been proposed in [25].

Our goal is to use the tools developed in [28, 25] to prove the relaxation to equilibrium of discrete versions of the Peierls model (1.7), whose collision operator is C_{12} . Similarly, we will prove the relaxation to equilibrium of the quantum Boltzmann model of the thermal cloud (1.1), whose collision operator is $C_{12} + C_{22}$, and modified quantum Boltzmann model of the thermal cloud (1.8), whose collision operator is $C_{12} + C_{22} + C_{13}$.

Notice that our relaxation to equilibrium results also agree with results from physics [76, 55, 54]. On the other hand, it was proved in [37], that (1.6) has a blow-up solution. However, the initial condition which creates blow-up solutions is concentrated around $p = 0$, which does not correspond to the high temperature regime of the thermal cloud under investigation here. Moreover, the discrete models considered here are the usual ones obtained from the derivations of these physical systems: for example, see equations (A23) and (A27) of [88] for C_{12} and C_{22} .

The plan of our paper is the following:

- In section 2, we show that the discrete version of equation (1.7) could be rewritten as a chemical reaction network. By using an approach inspired by the theory of toric dynamical system, we prove in Theorem 2.1. that the solution of the discrete version of (1.7) converges to the equilibrium exponentially in time.
- In section 3, we generalize Theorem 2.1 to collision operators of the forms C_{13} and C_{22} . We prove that the solutions of the discrete versions of these equations, associated with the collision operators C_{13} and C_{22} converge to equilibria exponentially in Theorems 3.1 and 3.2. In the case of C_{22} , we consider a one-dimensional version of the model.
- In Theorem 4.1 of Section 4, we extend Theorem 3.2 to the quantum Boltzmann model of the thermal cloud (1.1), and the modified quantum Boltzmann model of the thermal cloud (1.8).

2 A reaction network approach for the case of C_{12}

2.1 The dynamical system associated to C_{12}

As mentioned in the introduction, the model derived from physics to describe the system that couples BEC-excitations at very low temperature (and phonon interactions in anharmonic crystals) is the discrete version of (1.7) described below.

Let \mathcal{L}_R denote the lattice of integer points

$$\mathcal{L}_R = \{p \in \mathbb{Z}^3, |p| < R\}.$$

The discrete version of the quantum Boltzmann equation (1.7) reads

$$\begin{aligned} \dot{f}_{p_1} = & \sum_{\substack{p_2, p_3 \in \mathcal{L}_R, \\ p_1 - p_2 - p_3 = 0, \\ \mathcal{E}(p_1) - \mathcal{E}(p_2) - \mathcal{E}(p_3) = 0}} \mathcal{K}_{p_1, p_2, p_3}^{12} \{ (f_{p_1} + 1) f_{p_2} f_{p_3} - f_{p_1} (f_{p_2} + 1) (f_{p_3} + 1) \} \\ & - 2 \sum_{\substack{p_2, p_3 \in \mathcal{L}_R, \\ p_1 + p_2 - p_3 = 0, \\ \mathcal{E}(p_1) + \mathcal{E}(p_2) - \mathcal{E}(p_3) = 0}} \mathcal{K}_{p_1, p_2, p_3}^{12} \{ (f_{p_3} + 1) f_{p_1} f_{p_2} - f_{p_3} (f_{p_1} + 1) (f_{p_2} + 1) \}, \end{aligned} \quad (2.1)$$

for all p_1 in \mathcal{L}_R , where $\mathcal{E}(p)$ is defined in (1.5).

2.2 Decoupling the quantum Boltzmann equation associated to C_{12}

Note that when $p_1 = 0$, $\mathcal{K}_{p_1, p_2, p_3}^{12}$ is also 0, and therefore, we get

$$\dot{f}_0 = 0, \quad (2.2)$$

which says that $f_0(t)$ is a constant for all time t . Moreover, f_{p_1} does not depend on f_0 for all $p_1 \neq 0$. Therefore, without loss of generality, we can suppose that $f_0(0) = 0$, which leads to $f_0(t) = 0$ for all t .

Taking into account the fact $\mathcal{E}(p) = c|p|$, note that if $p_1, p_2, p_3 \in \mathcal{L}_R$ are different from 0 and $p_3 = p_1 + p_2$ and $|p_3| = |p_1| + |p_2|$ (like in the second sum of (2.1)), then p_1, p_2, p_3 must be collinear and on the same side of the origin. Therefore, we infer that there exists a vector P and $k_1, k_2, k_3 > 0$, $k_1, k_2, k_3 \in \mathbb{Z}$ such that

$$p_1 = k_1 P; \quad p_2 = k_2 P; \quad p_3 = k_3 P, \quad k_1 + k_2 = k_3.$$

Since \mathcal{L}_R is bounded, it follows that k_1, k_2, k_3 belong to a finite set of integer indices $\mathbb{I} = \{1, \dots, I\}$. Arguing similarly for the first sum in (2.1), we deduce that (2.1) is equivalent with the following system for $k_1 \in \mathbb{I}$

$$\begin{aligned} \dot{f}_{Pk_1} = & \sum_{\substack{k_2, k_3 \in \mathbb{I}, \\ k_1 - k_2 - k_3 = 0}} \mathcal{K}_{Pk_1, Pk_2, Pk_3}^{12} \{ (f_{Pk_1} + 1) f_{Pk_2} f_{Pk_3} - f_{Pk_1} (f_{Pk_2} + 1) (f_{Pk_3} + 1) \} \\ & - 2 \sum_{\substack{k_2, k_3 \in \mathbb{I}, \\ k_1 + k_2 - k_3 = 0}} \mathcal{K}_{Pk_1, Pk_2, Pk_3}^{12} \{ (f_{Pk_3} + 1) f_{Pk_1} f_{Pk_2} - f_{Pk_3} (f_{Pk_1} + 1) (f_{Pk_2} + 1) \}. \end{aligned} \quad (2.3)$$

Note that the system of equations (2.3) shows a *decoupling* of the system of equations (2.1) along a ray $\{kP_0\}$ with $k > 0$ (see Figure 1). As a consequence, it is sufficient to study the system of equations (2.3) for a fixed value of P_0 , instead of the system of equations (2.1).

If we denote $f_{k_1 P_0}$ by f_{k_1} (with $k_1 \in \mathbb{I}$) and $\mathcal{K}_{k_1 P_0, k_2 P_0, k_3 P_0}^{12}$ by $\mathcal{K}_{k_1, k_2, k_3}^{12}$, with an abuse

of notation, we obtain the following new system for the ray $\{k_1 P_0 | k_1 > 0\}$:

$$\begin{aligned} \dot{f}_{k_1} = & \sum_{\substack{k_2, k_3 \in \mathbb{I}, \\ k_1 = k_2 + k_3}} \mathcal{K}_{k_1, k_2, k_3}^{12} \{(f_{k_1} + 1) f_{k_2} f_{k_3} - f_{k_1} (f_{k_2} + 1) (f_{k_3} + 1)\} \\ & - 2 \sum_{\substack{k_2, k_3 \in \mathbb{I}, \\ k_1 + k_2 = k_3}} \mathcal{K}_{k_1, k_2, k_3}^{12} \{(f_{k_3} + 1) f_{k_1} f_{k_2} - f_{k_3} (f_{k_1} + 1) (f_{k_2} + 1)\}, \quad \forall k_1 \in \mathbb{I}. \end{aligned} \quad (2.4)$$

A simple calculation leads to the following *conservation of energy*

$$\sum_{k=1}^I k \dot{f}_k = 0, \quad (2.5)$$

or equivalently

$$\sum_{k=1}^I k f_k = \text{const.} \quad (2.6)$$

Also by abuse of notation, we denote this discrete version of C_{12} by

$$\begin{aligned} \mathcal{C}_{12}[f_{k_1}] := & \sum_{k_2 + k_3 = k_1} \mathcal{K}_{k_1, k_2, k_3}^{12} [(f_{k_1} + 1) f_{k_2} f_{k_3} - f_{k_1} (f_{k_2} + 1) (f_{k_3} + 1)] \\ & - 2 \sum_{k_1 + k_3 = k_2} \mathcal{K}_{k_2, k_1, k_3}^{12} [(f_{k_2} + 1) f_{k_1} f_{k_3} - f_{k_2} (f_{k_1} + 1) (f_{k_3} + 1)]. \end{aligned} \quad (2.7)$$

2.3 The chemical reaction network associated to C_{12}

For $x \in \mathbb{R}_{>0}^n$ and $\alpha \in \mathbb{R}_{\geq 0}^n$, we denote by x^α the monomial $\prod_{i=1}^n x_i^{\alpha_i}$.

Definition 2.1 *Consider a chemical reaction of the form*

$$\alpha_1 X_1 + \alpha_2 X_2 + \cdots + \alpha_n X_n \xrightarrow{\mathcal{K}} \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_n X_n,$$

where \mathcal{K} is a positive parameter, called reaction rate constant. Then the mass-action dynamical system generated by this reaction is

$$\dot{x} = \mathcal{K} x^\alpha (\beta - \alpha), \quad (2.8)$$

where $\alpha = (\alpha_1, \dots, \alpha_n)^T$, $\beta = (\beta_1, \dots, \beta_n)^T$, $\alpha_i, \beta_i > 0$ and $x = (x_1, \dots, x_n)^T$, in which x_i is the concentration of the chemical species X_i . For the case of a network that contains several reactions

$$\alpha_1^j X_1^j + \alpha_2^j X_2^j + \cdots + \alpha_n^j X_n^j \xrightarrow{\mathcal{K}_j} \beta_1^j X_1^j + \beta_2^j X_2^j + \cdots + \beta_n^j X_n^j,$$

for $1 \leq j \leq m$, its associated mass-action dynamical system is given by

$$\dot{x} = \sum_{j=1}^m \mathcal{K}_j x^{\alpha^j} (\beta^j - \alpha^j). \quad (2.9)$$

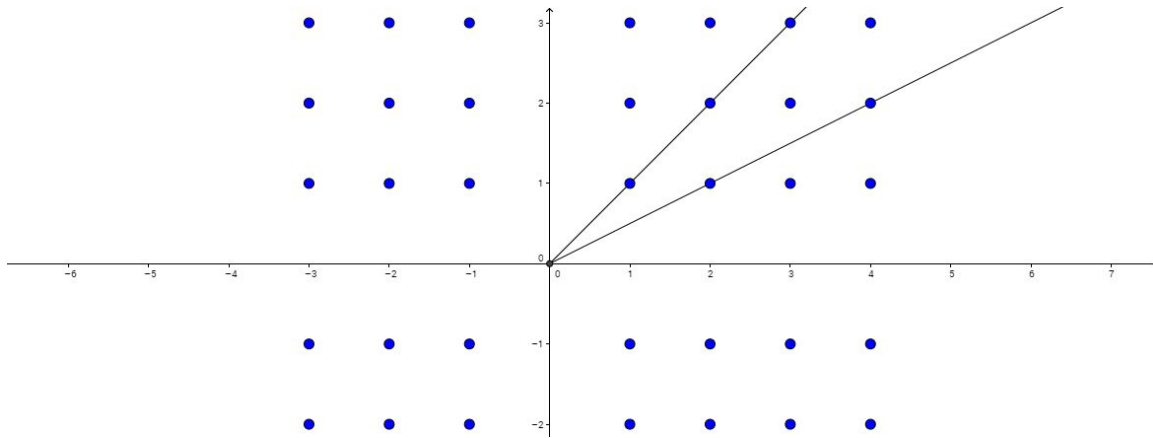
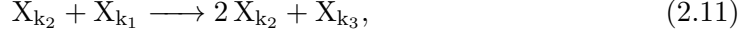


Figure 1: We decouple the systems into rays

In this section, we will show that the system (2.4) has the form (2.9) for a well-chosen set of reactions.

If $y \rightarrow y'$ and $y' \rightarrow y$ are reactions, we combine them together into a “reversible” reaction $y \leftrightarrow y'$.

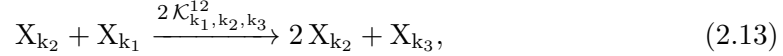
We will derive the system (2.4) from the network of chemical reactions of the form:



for all k_1, k_2, k_3 in \mathbb{I} such that $k_2 + k_3 = k_1$. If we denote by F_k the concentration of the species X_k , we will show that, for appropriate choices of the reaction rate constants in (2.10) and (2.11), the differential equations satisfied by F_k according the mass-action kinetics are exactly the same as (2.4).

In order to describe the connection between the mass-action system given by reactions of the form (2.10)-(2.11) and our system (2.4), we need to consider several cases.

Case 1: For $k_2 + k_3 = k_1$, $k_2 \neq k_3$, $k_1, k_2, k_3 \in \mathbb{I}$, we consider



and for the reversible reaction (2.12) the forward and backward rate constants are the same, i.e., we choose the reaction rate constants of the three reactions $X_{k_2} + X_{k_3} \rightarrow X_{k_1}$, $X_{k_1} \rightarrow X_{k_2} + X_{k_3}$, $X_{k_2} + X_{k_1} \rightarrow 2X_{k_2} + X_{k_3}$ to be $2\mathcal{K}_{k_1, k_2, k_3}^{12}$.

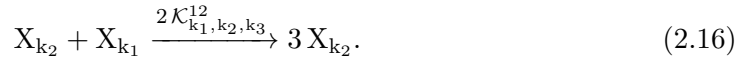
For example, consider the reversible reaction (2.12): in this reaction, X_{k_1} is created from $X_{k_2} + X_{k_3}$ with the rate $2\mathcal{K}_{k_1, k_2, k_3}^{12} F_{k_2} F_{k_3}$ and X_{k_1} is decomposed into $X_{k_2} + X_{k_3}$ with the rate $-2\mathcal{K}_{k_1, k_2, k_3}^{12} F_{k_1}$. Therefore, the rate of change of the species X_{k_1} due to this reaction is $2\mathcal{K}_{k_1, k_2, k_3}^{12} [F_{k_2} F_{k_3} - F_{k_1}]$.

For the irreversible reaction (2.13), X_{k_1} is lost with the rate $-2\mathcal{K}_{k_1, k_2, k_3}^{12} F_{k_2} F_{k_1}$ to create $2X_{k_2} + X_{k_3}$. Therefore the rate of change of the species X_{k_1} due to this reaction is $-2\mathcal{K}_{k_1, k_2, k_3}^{12} F_{k_2} F_{k_1}$. By exchanging the roles of X_{k_2} and X_{k_3} in (2.13), we obtain the rate $-2\mathcal{K}_{k_1, k_2, k_3}^{12} [F_{k_2} F_{k_1} + F_{k_3} F_{k_1}]$.

Therefore, the total rate of change of X_{k_1} due to the reactions in (2.12)-(2.13) is

$$2\mathcal{K}_{k_1, k_2, k_3}^{12} [F_{k_2} F_{k_3} - F_{k_1} - F_{k_2} F_{k_1} - F_{k_3} F_{k_1}]. \quad (2.14)$$

Case 2: For $2k_2 = k_1$, $k_1, k_2 \in \mathbb{I}$, we consider



We choose the reaction rate constant of $2X_{k_2} \rightarrow X_{k_1}$ and the reaction rate constant of $X_{k_1} \rightarrow 2X_{k_2}$ to be $\mathcal{K}_{k_1,k_2,k_3}^{12}$. Also, we choose the reaction rate constant of $X_{k_2} + X_{k_1} \rightarrow 3X_{k_2}$ to be $2\mathcal{K}_{k_1,k_2,k_3}^{12}$.

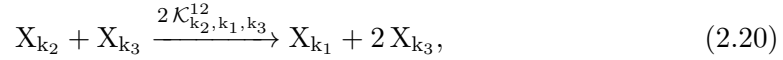
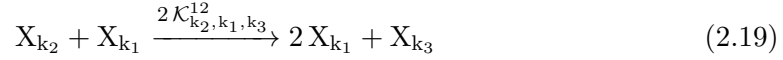
Consider the first reaction (2.15): In this reaction, X_{k_1} is created from $2X_{k_2}$ with the rate $\mathcal{K}_{k_1,k_2,k_2} F_{k_2}^2$ and X_{k_1} is decomposed into $2X_{k_2}$ with the rate $-\mathcal{K}_{k_1,k_2,k_2}^{12} F_{k_1}$. The rate of change of the species X_{k_1} is $\mathcal{K}_{k_1,k_2,k_2}^{12} [F_{k_2}^2 - F_{k_1}]$.

For the second reaction (2.16): X_{k_1} is lost with the rate $-2\mathcal{K}_{k_1,k_2,k_2}^{12} F_{k_2} F_{k_1}$ to create $3X_{k_2}$.

As a result, the rate of change of X_{k_1} due to the reactions (2.15)-(2.16) is

$$\mathcal{K}_{k_1,k_2,k_3}^{12} [F_{k_2}^2 - F_{k_1} - 2F_{k_2} F_{k_1}]. \quad (2.17)$$

Case 3: Next, for $k_2 = k_3 + k_1$, $k_1 \neq k_3$, $k_1, k_2, k_3 \in \mathbb{I}$, let us look at the rate of change of X_{k_1} in

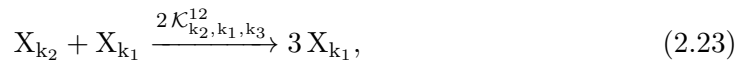


For (2.18), the rate of change of X_{k_1} is $2\mathcal{K}_{k_2,k_1,k_3}^{12} [F_{k_2} - F_{k_1} F_{k_3}]$. For (2.19), the rate of change of X_{k_1} is $2\mathcal{K}_{k_2,k_1,k_3}^{12} F_{k_1} F_{k_2}$. By exchanging the roles of X_1 and X_3 , we obtain the rate $2\mathcal{K}_{k_2,k_1,k_3}^{12} [F_{k_1} F_{k_2} + F_{k_2} F_{k_3}]$.

Therefore, the rate of change of X_{k_1} due to reactions in (2.18)-(2.20) is

$$-2\mathcal{K}_{k_2,k_1,k_3}^{12} [F_{k_1} F_{k_3} - F_{k_2} - F_{k_2} F_{k_3} - F_{k_1} F_{k_2}]. \quad (2.21)$$

Case 4: Now, for $k_2 = 2k_1$, $k_1, k_2 \in \mathbb{I}$, let us look at the rate of change of X_{k_1} in



For (2.22), the rate of change of X_{k_1} is $2\mathcal{K}_{k_2,k_1,k_3}^{12} [F_{k_2} - F_{k_1}^2]$. For (2.23), the rate of change of X_{k_1} is $4\mathcal{K}_{k_2,k_1,k_3}^{12} F_{k_1} F_{k_2}$. Therefore, the rate of change of X_{k_1} due to the reactions (2.22)-(2.23) is

$$-2\mathcal{K}_{k_2,k_1,k_3}^{12} [F_{k_1}^2 - F_{k_2} - 2F_{k_1} F_{k_2}]. \quad (2.24)$$

From (2.14), (2.17), (2.21), (2.24), the total rate of change of X_{k_1} is

$$\begin{aligned}
& \sum_{k_2+k_3=k_1, k_2 < k_3} 2\mathcal{K}_{k_1, k_2, k_3}^{12} [(F_{k_1} + 1)F_{k_2}F_{k_3} - F_{k_1}(F_{k_2} + 1)(F_{k_3} + 1)] \\
& + \sum_{2k_2=k_1} \mathcal{K}_{k_1, k_2, k_2}^{12} [(F_{k_1} + 1)F_{k_2}F_{k_2} - F_{k_1}(F_{k_2} + 1)(F_{k_2} + 1)] \\
& - \sum_{k_1+k_3=k_2} 2\mathcal{K}_{k_2, k_1, k_3}^{12} [(F_{k_2} + 1)F_{k_1}F_{k_3} - F_{k_2}(F_{k_1} + 1)(F_{k_3} + 1)],
\end{aligned} \tag{2.25}$$

which can be written as

$$\begin{aligned}
\dot{F}_{k_1} &= \sum_{k_2+k_3=k_1} \mathcal{K}_{k_1, k_2, k_3}^{12} [(F_{k_1} + 1)F_{k_2}F_{k_3} - F_{k_1}(F_{k_2} + 1)(F_{k_3} + 1)] \\
&- 2 \sum_{k_1+k_3=k_2} \mathcal{K}_{k_2, k_1, k_3}^{12} [(F_{k_2} + 1)F_{k_1}F_{k_3} - F_{k_2}(F_{k_1} + 1)(F_{k_3} + 1)],
\end{aligned} \tag{2.26}$$

which shows that the system of differential equations satisfied by the concentrations F_k is exactly the same as the system of differential equations (2.4) satisfied by the densities f_k .

2.4 A change of variables

In this section, we introduce a change of variables that will help us to investigate the dynamics of the system (2.26).

Define

$$G_k = \frac{F_k}{F_k + 1},$$

then

$$F_k = \frac{G_k}{1 - G_k},$$

and

$$\begin{aligned}
F_{k_3} + F_{k_1}F_{k_3} + F_{k_2}F_{k_3} - F_{k_1}F_{k_2} &= \frac{G_{k_3} - G_{k_1}G_{k_2}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})}, \\
F_{k_1} + F_{k_1}F_{k_2} + F_{k_1}F_{k_3} - F_{k_3}F_{k_2} &= \frac{G_{k_1} - G_{k_2}G_{k_3}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})}.
\end{aligned}$$

Notice that $0 < F_k < \infty$ and $0 < G_k < 1$.

The system (2.26) is converted into

$$\begin{aligned}
\frac{\dot{G}_{k_1}}{(1 - G_{k_1})^2} &= \tilde{\mathcal{C}}_{12}[G](k_1) := 2 \sum_{k_1+k_2=k_3} \mathcal{K}_{k_1, k_2, k_3}^{12} \frac{G_{k_3} - G_{k_1}G_{k_2}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})} \\
&+ \sum_{k_1=k_2+k_3} \mathcal{K}_{k_1, k_2, k_3}^{12} \frac{-G_{k_1} + G_{k_2}G_{k_3}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})}, \forall k_1 \in \mathbb{I}.
\end{aligned} \tag{2.27}$$

Suppose that G represents the column vector $(G_1, \dots, G_I)^T$. Let us also denote by X_k , with an abuse of notation, the vector

$$\begin{pmatrix} 0 \\ \dots \\ 1 \\ \dots \\ 0 \end{pmatrix},$$

in which the only element that different from 0 is the k -th one.

Also, for $k_1 \neq k_2$, we denote

$$\begin{aligned} K_{X_{k_1}+X_{k_2} \rightarrow X_{k_3}}(G) &:= 2\mathcal{K}_{k_1, k_2, k_3}^{12} \frac{G_{k_1} G_{k_2}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})}, \\ K_{X_{k_3} \rightarrow X_{k_1}+X_{k_2}}(G) &:= 2\mathcal{K}_{k_1, k_2, k_3}^{12} \frac{G_{k_3}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})}, \\ \mathcal{K}_{X_{k_1}+X_{k_2} \leftrightarrow X_{k_3}} &:= 2\mathcal{K}_{k_1, k_2, k_3}^{12}. \end{aligned}$$

Otherwise, if $k_1 = k_2$, we denote

$$\begin{aligned} K_{2X_{k_1} \rightarrow X_{k_3}}(G) &:= \mathcal{K}_{k_1, k_1, k_3}^{12} \frac{G_{k_1} G_{k_2}}{(1 - G_{k_1})^2(1 - G_{k_3})}, \\ K_{X_{k_3} \rightarrow 2X_{k_1}}(G) &:= \mathcal{K}_{k_1, k_1, k_3}^{12} \frac{G_{k_3}}{(1 - G_{k_1})^2(1 - G_{k_3})}, \\ \mathcal{K}_{2X_{k_1} \leftrightarrow X_{k_3}} &:= 2\mathcal{K}_{k_1, k_1, k_3}^{12}. \end{aligned}$$

Using these notations, the system (2.27) could be rewritten as:

$$\begin{aligned} \dot{G} &= \text{diag} \begin{pmatrix} (1 - G_1)^2 \\ \dots \\ (1 - G_I)^2 \end{pmatrix} \times \\ &\times \sum_{k_1+k_2=k_3} \left[K_{X_{k_1}+X_{k_2} \rightarrow X_{k_3}}(G) - K_{X_{k_3} \rightarrow X_{k_1}+X_{k_2}}(G) \right] (X_{k_3} - X_{k_1} - X_{k_2}). \end{aligned} \quad (2.28)$$

Equivalently, we can also write

$$\dot{G} = \text{diag} \begin{pmatrix} (1 - G_1)^2 \\ \dots \\ (1 - G_I)^2 \end{pmatrix} \sum_{y \leftrightarrow y'} \left[K_{y \rightarrow y'}(G) - K_{y' \rightarrow y}(G) \right] (y' - y), \quad (2.29)$$

where $y \leftrightarrow y'$ belongs to the set of reversible reactions

$$X_{k_1} + X_{k_2} \longleftrightarrow X_{k_3}, \quad (2.30)$$

with $k_1 + k_2 = k_3$.

2.5 Convergence to equilibrium

Theorem 2.1 *For any positive initial condition, the solution*

$$f(t) = (f_p(t))_{p \in \mathcal{L}_R}$$

of the discrete quantum Boltzmann equation (2.1) converges to an equilibrium state $f^ = (f_p^*)_{p \in \mathcal{L}_R}$. For each ray $\{kP_0\}_{k \geq 1}$ there exists a positive constant $\rho(P_0)$ such that if $p = kP_0$ then*

$$f_p^* = \frac{1}{e^{k\rho(P_0)} - 1}.$$

Moreover, the solution $f(t)$ of (2.1) converges to f^ exponentially fast in the following sense: there exist positive constants C_1, C_2 such that*

$$\max_{p \in \mathcal{L}_R} |f_p(t) - f_p^*| < C_1 e^{-C_2 t}.$$

Proof By using the decoupling and the change of variables discussed in the previous sections, for each ray $\{kP_0\}_{k \geq 1}$, we can reduce the study of f to F , which satisfies (2.26). From F , we can switch to study G , which is the solution of (2.29).

Step 1: The Lyapunov function. We recall that (2.27) could be rewritten under the form

$$\dot{G} = \text{diag} \begin{pmatrix} (1 - G_1)^2 \\ \vdots \\ (1 - G_I)^2 \end{pmatrix} \sum_{y \leftrightarrow y'} [K_{y \rightarrow y'}(G) - K_{y' \rightarrow y}(G)] (y' - y). \quad (2.31)$$

We define the function

$$L(G) = \sum_{k=1}^I \log(1 - G_k) + \frac{G_k \log G_k}{1 - G_k} - \frac{\log G_k^*}{1 - G_k}, \quad (2.32)$$

where $G_k^* = \frac{1}{e^{k\rho}}$, for some $\rho > 0$, and we will show that L is a Lyapunov function for the system (2.27).

We have

$$\nabla L = \begin{pmatrix} \frac{1}{(1-G_1)^2} \log \frac{G_1}{G_1^*} \\ \vdots \\ \frac{1}{(1-G_I)^2} \log \frac{G_I}{G_I^*} \end{pmatrix}, \quad (2.33)$$

which implies that

$$\begin{aligned} \text{diag} \begin{pmatrix} (1 - G_1)^2 \\ \vdots \\ (1 - G_I)^2 \end{pmatrix} \cdot (y' - y) \cdot \nabla L &= \log \left(\frac{G}{G^*} \right)^{y' - y} \\ &= \log \left(\frac{G}{G^*} \right)^{y'} - \log \left(\frac{G}{G^*} \right)^y. \end{aligned} \quad (2.34)$$

If we define

$$\mathcal{H}_{y,y'}(G) = \frac{K_{y \rightarrow y'}(G)}{\mathcal{K}_{y \leftrightarrow y'} G^y},$$

then $\mathcal{H}_{y,y'} = \mathcal{H}_{y',y}$ for y and y' as in (2.30). Moreover, we have

$$\begin{aligned} & K_{y \rightarrow y'}(G) - K_{y' \rightarrow y}(G) = \\ &= \mathcal{K}_{y \leftrightarrow y'} G^y \mathcal{H}_{y,y'}(G) - \mathcal{K}_{y \leftrightarrow y'} G^{y'} \mathcal{H}_{y,y'}(G) \\ &= \mathcal{K}_{y \leftrightarrow y'} \mathcal{H}_{y,y'}(G) [G^y - G^{y'}] \\ &= \mathcal{K}_{y \leftrightarrow y'} (G^*)^y \mathcal{H}_{y,y'}(G) \left[\frac{G^y}{(G^*)^y} - \frac{G^{y'}}{(G^*)^{y'}} \right], \end{aligned} \tag{2.35}$$

since $(G^*)^y = (G^*)^{y'}$.

Combining (2.31), (2.34) and (2.35), we obtain

$$\begin{aligned} & \dot{G} \cdot \nabla L = \\ &= \sum_{y \leftrightarrow y'} \left[\log \left(\frac{G}{G^*} \right)^{y'} - \log \left(\frac{G}{G^*} \right)^y \right] \mathcal{K}_{y \leftrightarrow y'} (G^*)^y \mathcal{H}_{y,y'}(G) \left[\frac{G^y}{(G^*)^y} - \frac{G^{y'}}{(G^*)^{y'}} \right] \\ &\leq 0, \end{aligned} \tag{2.36}$$

since log is an increasing function. Also, note that the above inequality is strict unless

$$\frac{G^y}{(G^*)^y} = \frac{G^{y'}}{(G^*)^{y'}}, \tag{2.37}$$

for all reactions $y \leftrightarrow y'$.

Since $(G^*)^y = (G^*)^{y'}$ for all reactions $y \leftrightarrow y'$, this implies $G_{k_1}^* \cdot G_{k_2}^* = G_{k_1+k_2}^*$ for all k_1 and k_2 such that $k_1 + k_2 \leq I$. As a consequence $G_k^* = e^{-\rho k}$, for some positive constant ρ . Moreover, (2.37) implies that at equilibrium $(G)^y = (G)^{y'}$ for all reactions $y \leftrightarrow y'$, which leads to $G_k = e^{-\rho' k}$, for some positive constant ρ' .

By the conservation relation

$$\sum_{k=1}^I k \frac{G_k}{1 - G_k} = \sum_{k=1}^I k \frac{G_k^*}{1 - G_k^*},$$

we deduce that

$$\sum_{k=1}^I k \frac{e^{-\rho k}}{1 - e^{-\rho k}} = \sum_{k=1}^I k \frac{e^{-\rho' k}}{1 - e^{-\rho' k}}.$$

By the monotonicity of the function $\rho \rightarrow \frac{e^{-\rho k}}{1 - e^{-\rho k}}$, we conclude that $\rho = \rho'$, i.e., G^* is the only equilibrium point that satisfies the same conservation relation as the initial condition.

Now, we will prove that there exists exactly one critical point of the Lyapunov function L within each invariant set

$$\mathfrak{S}_c := \left\{ \sum_{k=1}^I k \frac{G_k}{1-G_k} = c \right\}.$$

Since

$$\nabla L = \text{diag} \begin{pmatrix} \frac{1}{(1-G_1)^2} \\ \cdots \\ \frac{1}{(1-G_I)^2} \end{pmatrix} [\log G - \log G^*],$$

the projection of ∇L on the tangent space to the set \mathfrak{S}_c is 0 if and only if there exists a constant ϱ such that

$$\nabla L = \varrho \cdot \nabla \left(\sum_{k=1}^I k \frac{G_k}{1-G_k} \right),$$

which is equivalent with

$$\text{diag} \begin{pmatrix} \frac{1}{(1-G_1)^2} \\ \cdots \\ \frac{1}{(1-G_I)^2} \end{pmatrix} [\log G - \log G^*] = \varrho \begin{pmatrix} \frac{1}{(1-G_1)^2} \\ \cdots \\ \frac{1}{(1-G_I)^2} \end{pmatrix}.$$

A direct consequence of the above is the following system of identities

$$\begin{aligned} \log G_1 - \log G_1^* &= \varrho, \\ \log G_2 - \log G_2^* &= \varrho, \\ &\cdots \\ \log G_I - \log G_I^* &= \varrho, \end{aligned}$$

yielding

$$\frac{G_k}{G_k^*} = e^{k\varrho}, \quad \forall k \in \{1, \dots, I\}.$$

Moreover, since G_k and G_k^* satisfy the same conservation law then it follows that $G = G^*$. This implies that G^* is the only critical point of L on the invariant set \mathfrak{S}_c .

Step 2: Differential inclusions and persistence. Now let us observe that (2.4) could be regarded as a \mathcal{K} -variable mass-action system for the reversible network (2.30). For this we write

$$F_{k''} + F_k F_{k''} + F_{k'} F_{k''} = (1 + F_k + F_{k'}) F_{k''},$$

and note that $1 + F_k + F_{k'}$ is bounded below by 1 and above by $1 + 2C$, where

$$C = \sum_{k=1}^I k F_k.$$

Therefore, the results of [25] about persistence of \mathcal{K} -variable reversible mass-action systems can be applied and we conclude that the system is persistent. Alternatively, we can also use the Petri net argument of [8], to prove that the system is persistent, as follows. Note that F_k is the density function of the species X_k . It is straightforward that each *siphon* is $\{X_1, X_2, \dots, X_I\}$, which contains the support of the *P-semiflow* (see [8] for the definition of siphons and P-semiflows) given by

$$\sum_{k=1} k F_k = \text{constant}.$$

As a result, the Petri net theory developed in [8] can be applied and it follows that the system is persistent.

Therefore, by using the existence of the globally defined strict Lyapunov function L , and the LaSalle invariance principle, it follows that all trajectories converge to the unique positive equilibrium G^* that we discussed in Step 1.

Step 3: Exponential rate of convergence. Define

$$\begin{aligned} \mathcal{R}(G) &= \\ &= \text{diag} \begin{pmatrix} (1 - G_1)^2 \\ \cdots \\ (1 - G_I)^2 \end{pmatrix} \sum_{y \leftrightarrow y'} [K_{y \rightarrow y'}(G) - K_{y' \rightarrow y}(G)] (y' - y) \\ &= \text{diag} \begin{pmatrix} (1 - G_1)^2 \\ \cdots \\ (1 - G_I)^2 \end{pmatrix} \sum_{y \leftrightarrow y'} [\mathcal{K}_{y \leftrightarrow y'} G^y - \mathcal{K}_{y \leftrightarrow y'} G^{y'}] \mathcal{H}_{y, y'}(G) (y' - y), \end{aligned} \quad (2.38)$$

and define

$$\mathcal{S}(G) = \sum_{y \leftrightarrow y'} [\mathcal{K}_{y \leftrightarrow y'} G^y - \mathcal{K}_{y \leftrightarrow y'} G^{y'}] \mathcal{H}_{y, y'}(G) (y' - y).$$

Following [27], we compute the Jacobian of \mathcal{S} at the equilibrium point G^* , applied to an arbitrary vector $\delta \neq 0$ that belongs to the span of the vectors $y' - y$

$$\text{Jac}(\mathcal{S}(G^*))\delta = \sum_{y \leftrightarrow y'} \mathcal{K}_{y \leftrightarrow y'}(G^*)^y ((y - y') * \delta) \mathcal{H}_{y, y'}(G^*)(y - y'), \quad (2.39)$$

in which the inner product $*$ is defined as

$$y * \delta = \sum_1^I \frac{y_k \delta_k}{G_k}.$$

Therefore

$$[\text{Jac}(\mathcal{S}(G^*))\delta] * \delta = \quad (2.40)$$

$$= \sum_{y \leftrightarrow y'} \mathcal{K}_{y \leftrightarrow y'}(G^*)^y \mathcal{H}_{y, y'}(G^*) [(y - y') * \delta] [(y' - y) * \delta] < 0.$$

Now, we compute the Jacobian of \mathcal{R} at the equilibrium point G^* ,

$$\begin{aligned} & \text{Jac}(\mathcal{R}(G^*)) \\ &= \text{diag} \begin{bmatrix} \partial_{G_1}(1 - G_1^*)^2 \mathcal{S}(G^*)_1 \\ \cdots \\ \partial_{G_I}(1 - G_I^*)^2 \mathcal{S}(G^*)_I \end{bmatrix} + \text{diag} \begin{bmatrix} (1 - G_1^*)^2 \\ \cdots \\ (1 - G_I^*)^2 \end{bmatrix} \text{Jac}(\mathcal{S}(G^*)) \\ &= \text{diag} \begin{bmatrix} (1 - G_1^*)^2 \\ \cdots \\ (1 - G_I^*)^2 \end{bmatrix} \text{Jac}(\mathcal{S}(G^*)), \end{aligned}$$

where the second equality is due to the fact that since G^* is an equilibrium we have that $\mathcal{S}(G^*) = 0$.

Since

$$D := \text{diag} \begin{bmatrix} (1 - G_1^*)^2 \\ \cdots \\ (1 - G_I^*)^2 \end{bmatrix}$$

is a diagonal matrix with respect to the inner product $*$ and $A := \text{Jac}(\mathcal{S}(G^*))$ is negative definite with respect to the inner product $*$, then $D^{1/2}AD^{1/2}$ is also negative definite with respect to this inner product. Since

$$\det(DA - \lambda Id) = \det(D^{1/2}AD^{1/2} - \lambda Id), \quad \forall \lambda \in \mathbb{R},$$

it follows that $D^{1/2}AD^{1/2}$ and DA have the same eigenvectors, so DA is negative definite. In other words, $\text{Jac}(\mathcal{R}(G^*))$ is negative definite. The exponential rate of convergence

$$\max\{|G_1(t) - G_1^*|, \dots, |G_I(t) - G_I^*|\} \leq C_1 e^{-C_2 t}.$$

then follows from the fact that the Jacobian above is negative definite. This leads to the conclusion of our theorem. ■

Remark 2.1 *The Lyapunov function (2.32) in the variable F reads*

$$L(F) = \sum_{k=1}^I [F_k \log F_k - (1 + F_k) \log(1 + F_k) + (\log(F_k^* + 1) - \log F_k^*)(F_k + 1)], \quad (2.41)$$

and it is a strictly convex function.

Remark 2.2 *If the intersection between the ray $\{kP_0\}_{k \geq 1}$ and \mathcal{L}_R contains a single point, then the solution $f(t)$ of (2.1) has $f_{P_0} \equiv 0$, so $f_{P_0} \equiv \text{constant}$.*

3 A reaction network approach for the case of C_{13} and C_{22}

3.1 The dynamical system associated to C_{13}

As we discussed in the Introduction, we are also interested in the dynamics given by the discrete model of the collision operator C_{13} , described in (1.9).

Let \mathcal{L}_R denote the lattice of integer points

$$\mathcal{L}_R = \{p \in \mathbb{Z}^3 \mid |p| < R\}.$$

The discretized quantum Boltzmann equation for C_{13} reads

$$\begin{aligned} \dot{f}_{p_1} &= C_{13}^D[f_{p_1}] := \\ &:= \sum_{\substack{p_2, p_3, p_4 \in \mathcal{L}_R, \\ p_1 = p_2 + p_3 + p_4, \\ \mathcal{E}(p_1) = \mathcal{E}(p_2) + \mathcal{E}(p_3) + \mathcal{E}(p_4)}} \mathcal{K}_{p_1, p_2, p_3, p_4}^{13} \{ (f_{p_1} + 1) f_{p_2} f_{p_3} f_{p_4} - (f_{p_2} + 1)(f_{p_3} + 1)(f_{p_4} + 1) f_{p_1} \} \\ &\quad - 3 \sum_{\substack{p_2, p_3, p_4 \in \mathcal{L}_R, \\ p_2 = p_1 + p_3 + p_4, \\ \mathcal{E}(p_2) = \mathcal{E}(p_1) + \mathcal{E}(p_3) + \mathcal{E}(p_4)}} \mathcal{K}_{p_2, p_1, p_3, p_4}^{13} \{ (f_{p_2} + 1) f_{p_1} f_{p_3} f_{p_4} - (f_{p_1} + 1)(f_{p_3} + 1)(f_{p_4} + 1) f_{p_2} \}, \end{aligned} \quad (3.1)$$

for all p_1 in \mathcal{L}_R , where $\mathcal{E}(p)$ is defined in (1.5).

Similar to the C_{12} case, when $p = 0$, $\mathcal{K}_{p_1, p_2, p_3, p_4}^{13} = 0$, and we obtain

$$\dot{f}_0 = 0,$$

which means $f_0(t)$ is a constant for all time t , and we can assume $f_0(t) = 0$ for all t .

Since in the first sum of (3.1), we consider (p_1, p_2, p_3, p_4) satisfying

$$p_1 = p_2 + p_3 + p_4, \quad \mathcal{E}(p_1) = \mathcal{E}(p_2) + \mathcal{E}(p_3) + \mathcal{E}(p_4), \quad (3.2)$$

we infer that there exists a vector P and $k_1, k_2, k_3, k_4 \geq 0$, $k_1, k_2, k_3, k_4 \in \mathbb{Z}$ such that

$$p_1 = k_1 P; \quad p_2 = k_2 P; \quad p_3 = k_3 P; \quad p_4 = k_4 P; \quad k_1 = k_2 + k_3 + k_4.$$

Using the same arguments as the case of C_{12} , we can deduce that Equation (3.1) for C_{13} is equivalent with the following family of decoupled systems for $k_1 \in \mathbb{I} = \{1, 2, \dots, I\}$ where P is the closest point to the origin among the lattice points on its ray:

$$\begin{aligned} \dot{f}_{k_1 P} &= \\ &= \sum_{\substack{k_2, k_3, k_4 \in \mathbb{I}, \\ k_1 = k_2 + k_3 + k_4}} \mathcal{K}_{k_1 P, k_2 P, k_3 P, k_4 P}^{13} \{ (f_{k_1 P} + 1) f_{k_2 P} f_{k_3 P} f_{k_4 P} \\ &\quad - f_{k_1 P} (f_{k_2 P} + 1)(f_{k_3 P} + 1)(f_{k_4 P} + 1) \} \\ &\quad - 3 \sum_{\substack{k_2, k_3, k_4 \in \mathbb{I}, \\ k_2 = k_1 + k_3 + k_4}} \mathcal{K}_{k_2 P, k_1 P, k_3 P, k_4 P}^{13} \{ (f_{k_2 P} + 1) f_{k_1 P} f_{k_3 P} f_{k_4 P} \\ &\quad - f_{k_2 P} (f_{k_1 P} + 1)(f_{k_3 P} + 1)(f_{k_4 P} + 1) \}. \end{aligned} \quad (3.3)$$

Denoting f_{kP} by F_k (with $k \in \mathbb{I}$) and $\mathcal{K}_{k_1P, k_2P, k_3P, k_4P}^{12}$ by $\mathcal{K}_{k_1, k_2, k_3, k_4}^{12}$, we obtain

$$\begin{aligned} \dot{F}_{k_1} = \mathcal{C}_{13}[F](k_1) = & \sum_{k_1=k_2+k_3+k_4} \mathcal{K}_{k_1, k_2, k_3, k_4}^{13} \{ (F_{k_1} + 1)F_{k_2}F_{k_3}F_{k_4} - \\ & - F_{k_1}(F_{k_2} + 1)(F_{k_3} + 1)(F_{k_4} + 1) \} \\ & - 3 \sum_{k_1+k_2+k_3=k_4} \mathcal{K}_{k_1, k_2, k_3, k_4}^{13} \{ (F_{k_4} + 1)F_{k_1}F_{k_2}F_{k_3} - \\ & - F_{k_4}(F_{k_1} + 1)(F_{k_2} + 1)(F_{k_3} + 1) \}, \quad \forall k_1 \in \mathbb{I}. \end{aligned} \quad (3.4)$$

In order to ensure that all the variables F_k are coupled with each other, let us assume that $I \geq 4$. We have the following conservation of energy for C_{13}

$$\sum_{k=1}^I k \dot{F}_k = 0, \quad (3.5)$$

or equivalently

$$\sum_{k=1}^I k F_k = \text{const.} \quad (3.6)$$

Similar to the case of C_{12} , we define

$$G_k = \frac{F_k}{F_k + 1},$$

and then we have

$$F_k = \frac{G_k}{1 - G_k}.$$

Note that, similar to the previous section, $0 < F_k < \infty$ and $0 < G_k < 1$.

The system (3.4) can be now written

$$\begin{aligned} \frac{\dot{G}_{k_1}}{(1 - G_{k_1})^2} = \overline{\mathcal{C}}_{13}[G] := & \mathcal{K}_{k_1, k_2, k_3, k_4}^{13} \sum_{\substack{k_1=k_2+k_3+k_4, \\ |k_1|=|k_2|+|k_3|+|k_4|}} \frac{G_{k_2}G_{k_3}G_{k_4} - G_{k_1}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})(1 - G_{k_4})} \\ & - 3\mathcal{K}_{k_2, k_1, k_3, k_4}^{13} \sum_{\substack{k_2=k_1+k_3+k_4, \\ |k_2|=|k_1|+|k_3|+|k_4|}} \frac{G_{k_1}G_{k_3}G_{k_4} - G_{k_2}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})(1 - G_{k_4})}. \end{aligned} \quad (3.7)$$

This system can also be rewritten as

$$\begin{aligned} \dot{G} = & \text{diag} \begin{pmatrix} (1 - G_1)^2 \\ \cdots \\ (1 - G_I)^2 \end{pmatrix} \times \\ & \times \sum_{\substack{k_1=k_2+k_3+k_4, \\ |k_1|=|k_2|+|k_3|+|k_4|}} [K_{X_{k_2}+X_{k_3}+X_{k_4} \rightarrow X_{k_1}}(G) - K_{X_{k_1} \rightarrow X_{k_2}+X_{k_3}+X_{k_4}}(G)] (X_{k_1} - X_{k_2} - X_{k_3} - X_{k_4}). \end{aligned} \quad (3.8)$$

where X_k is, with an abuse of notation, as mentioned earlier, the vector

$$\begin{pmatrix} 0 \\ \cdots \\ 1 \\ \cdots \\ 0 \end{pmatrix},$$

in which the only element that is 1 is the k -th one, and

$$\begin{aligned} K_{X_{k_2}+X_{k_3}+X_{k_4} \rightarrow X_{k_1}}(G) &:= \mathcal{K}_{k_1, k_2, k_3, k_4}^{13} \frac{G_{k_1}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})(1 - G_{k_4})}, \\ K_{X_{k_1} \rightarrow X_{k_2}+X_{k_3}+X_{k_4}}(G) &:= \mathcal{K}_{k_1, k_2, k_3, k_4}^{13} \frac{G_{k_2} G_{k_3} G_{k_4}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})(1 - G_{k_4})}. \end{aligned}$$

We can also write

$$\dot{G} = \text{diag} \begin{pmatrix} (1 - G_1)^2 \\ \cdots \\ (1 - G_I)^2 \end{pmatrix} \sum_{y \leftrightarrow y'} [K_{y \rightarrow y'}(G) - K_{y' \rightarrow y}(G)] (y' - y),$$

where $y \leftrightarrow y'$ rang over the reversible reactions shown above.

Theorem 3.1 *For any initial condition, the solution*

$$f(t) = (f_p(t))_{p \in \mathcal{L}_R}$$

of the quantum Boltzmann equation (3.1) converges to an equilibrium state $f^ = (f_p^*)_{p \in \mathcal{L}_R}$. For each ray $\{kP_0\}_{k \geq 1}$ that intersects \mathcal{L}_R in at least 4 points there exists a constant ρ_{P_0} such that if $p = kP_0$ then*

$$f_p^* = \frac{1}{e^{k\rho_{P_0}} - 1}.$$

Moreover, the solution $f(t)$ of (3.1) converges to f^ exponentially fast in the following sense: there exists positive constants C_1, C_2 such that*

$$\max_{p \in \mathcal{L}_R} |f_p(t) - f_p^*| < C_1 e^{-C_2 t}.$$

Proof The proof of Theorem 3.2 then follows exactly from the same Lyapunov function (2.32) and arguments as in Theorem 2.1. ■

3.2 The dynamical system associated to C_{22}

Let us consider a discretized version of the quantum Boltzmann model associated to the collision operator given by C_{22} :

Let \mathcal{L}_R denote the lattice of integer points

$$\mathcal{L}_R = \{p \mid |p| \in \mathbb{Z}^3, |p| < R\}.$$

The discretized quantum Boltzmann equation associated to C_{22} reads $\forall p_1 \in \mathcal{L}_R$

$$\begin{aligned} \dot{f}_{p_1} &= C_{22}^D[f_{p_1}] := \\ &:= \sum_{\substack{p_2, p_3, p_4 \in \mathcal{L}_R, \\ p_1 + p_2 = p_3 + p_4, \\ \mathcal{E}(p_1) + \mathcal{E}(p_2) = \mathcal{E}(p_3) + \mathcal{E}(p_4)}} \mathcal{K}_{p_1, p_2, p_3, p_4}^{13} \{(f_{p_1} + 1)(f_{p_2} + 1)f_{p_3}f_{p_4} - f_{p_1}f_{p_2}(f_{p_3} + 1)(f_{p_4} + 1)\}, \end{aligned} \quad (3.9)$$

where $\mathcal{E}(p)$ is defined in (1.5).

Similar to the C_{12} case, when $p = 0$, $\mathcal{K}_{p_1, p_2, p_3, p_4}^{22} = 0$, and we obtain

$$\dot{f}_0 = 0,$$

which means $f_0(t)$ is a constant for all time t . As a consequence, we can suppose that $f_0(0) = 0$, which implies $f_0(t) = 0$ for all t .

In (3.9), the sums for C_{22} are taken over (p_1, p_2, p_3, p_4) satisfying

$$p_1 + p_2 = p_3 + p_4, \text{ and } \mathcal{E}(p_1) + \mathcal{E}(p_2) = \mathcal{E}(p_3) + \mathcal{E}(p_4). \quad (3.10)$$

In this case, unlike in the case of C_{12} and C_{13} , we *cannot* infer from (3.10) that there exists a vector P and $k_1, k_2, k_3, k_4 \geq 0$, $k_1, k_2, k_3, k_4 \in \mathbb{Z}$ such that

$$p_1 = k_1 P; \quad p_2 = k_2 P; \quad p_3 = k_3 P; \quad p_4 = k_4 P, \quad k_1 + k_2 = k_3 + k_4.$$

However, let us consider the following simplified version of (3.9) for C_{22}

$$\begin{aligned} \dot{F}_{k_1} &= C_{22}[F](k_1) := \sum_{\substack{k_1 + k_2 = k_3 + k_4 \\ k_2, k_3, k_4 \in \mathbb{I}}} \mathcal{K}_{k_1, k_2, k_3, k_4}^{13} \{(F_{k_1} + 1)(F_{k_2} + 1)F_{k_3}F_{k_4} - \\ &- F_{k_1}F_{k_2}(F_{k_3} + 1)(F_{k_4} + 1)\}, \quad \forall k_1 \in \mathbb{I}. \end{aligned} \quad (3.11)$$

Recall that $\mathbb{I} = \{1, \dots, I\}$. We also suppose that $I \geq 3$. We have the following conservation of energy

$$\sum_{k=1}^I k \dot{F}_k = 0, \quad (3.12)$$

or equivalently

$$\sum_{k=1}^I k F_k = \text{const.} \quad (3.13)$$

For C_{22} , the following “conservation of mass” also holds

$$\sum_{k=1}^I \dot{F}_k = 0, \quad (3.14)$$

or equivalently

$$\sum_{k=1}^I F_k = \text{const.} \quad (3.15)$$

Similar to the case of C_{12} , define

$$G_k = \frac{F_k}{F_k + 1},$$

then

$$F_k = \frac{G_k}{1 - G_k},$$

and the system (3.9) can be now written

$$\begin{aligned} \frac{\dot{G}_{k_1}}{(1 - G_{k_1})^2} &= \overline{\mathcal{C}_{22}}[G] := \\ &:= \mathcal{K}_{k_1, k_2, k_3, k_4}^{13} \sum_{\substack{k_1 + k_2 = k_3 + k_4, \\ |k_1| + |k_2| = |k_3| + |k_4|}} \frac{G_{k_3} G_{k_4} - G_{k_1} G_{k_2}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})(1 - G_{k_4})}. \end{aligned} \quad (3.16)$$

This system can be rewritten as

$$\begin{aligned} \dot{G} &= \text{diag} \left(\begin{pmatrix} (1 - G_1)^2 \\ \vdots \\ (1 - G_I)^2 \end{pmatrix} \right) \times \\ &\times \sum_{\substack{k_1 + k_2 = k_3 + k_4, \\ |k_1| + |k_2| = |k_3| + |k_4|}} [K_{X_{k_3} + X_{k_4} \rightarrow X_{k_2} + X_{k_1}}(G) \\ &- K_{X_{k_2} + X_{k_1} \rightarrow X_{k_3} + X_{k_4}}(G)] (X_{k_1} + X_{k_2} - X_{k_3} - X_{k_4}). \end{aligned} \quad (3.17)$$

where X_k is, with an abuse of notation, the vector

$$\begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix},$$

in which the only element that is 1 is the k -th one, and

$$K_{X_{k_3} + X_{k_4} \rightarrow X_{k_2} + X_{k_1}}(G) = \mathcal{K}_{k_1, k_2, k_3, k_4}^{13} \frac{G_{k_1} G_{k_2}}{(1 - G_{k_1})(1 - G_{k_2})(1 - G_{k_3})(1 - G_{k_4})},$$

$$K_{X_{k_2}+X_{k_1} \rightarrow X_{k_3}+X_{k_4}}(G) = \mathcal{K}_{k_1,k_2,k_3,k_4}^{13} \frac{G_{k_3}G_{k_4}}{(1-G_{k_1})(1-G_{k_2})(1-G_{k_3})(1-G_{k_4})}.$$

We can also write

$$\dot{G} = \text{diag} \begin{pmatrix} (1-G_1)^2 \\ \cdots \\ (1-G_I)^2 \end{pmatrix} \sum_{y \leftrightarrow y'} [K_{y \rightarrow y'}(G) - K_{y' \rightarrow y}(G)] (y' - y),$$

where $y \leftrightarrow y'$ range over the reversible reactions shown above.

Theorem 3.2 *For any initial condition, the solution*

$$F(t) = (F_k(t))_{k \in \mathbb{I}}$$

of the quantum Boltzmann equation (3.11) converges to an equilibrium state $F^ = (F_k^*)_{k \in \mathbb{I}}$, where*

$$F_k^* = \frac{1}{e^{\rho_2(k-1) - \rho_1(k-2)} - 1}.$$

Moreover, the solution $F(t)$ of (3.11) converges to F^ exponentially fast in the following sense: there exists positive constants C_1, C_2 such that*

$$\max_{k \in \mathbb{I}} |F_k(t) - F_k^*| < C_1 e^{-C_2 t}.$$

Proof We notice that

$$\frac{G^y}{(G^*)^y} = \frac{G^{y'}}{(G^*)^{y'}}, \quad (3.18)$$

holds true for all reactions $y \leftrightarrow y'$, if and only if since $(G^*)^y = (G^*)^{y'}$ for all reactions $y \leftrightarrow y'$. In the case of C_{22} , we obtain the relation $G_{k_1}^* \cdot G_{k_2}^* = G_{k_3}^* \cdot G_{k_4}^*$ for all k_1, k_2, k_3, k_4 such that $k_1 + k_2 = k_3 + k_4 \leq I$. From the relation $G_{k_1} \cdot G_{k_2} = G_{k_3} \cdot G_{k_4}$ and the fact that $k + (k-2) = 2(k-1)$, the following identity holds true

$$G_k(G_1)^{k-2} = (G_2)^{k-1}.$$

We then obtain $G_k = (G_2)^{k-1}/(G_1)^{k-2}$. Identity (3.18) then implies that $(G)^y = (G)^{y'}$ for all reactions $y \leftrightarrow y'$, which leads to $G_k = e^{\rho' k}$.

The conservation relation

$$\sum_{k=1}^n \frac{G_k}{1-G_k} = \sum_{k=1}^n \frac{G_k^*}{1-G_k^*},$$

implies that that $\rho = \rho'$, then $G_k = G_k^*$.

We can still use the Petri net argument of [8] or the result in [25], to prove that the system is persistent. For example, to use the method from [8], we note that we have two *siphons* $\{X_1, X_2, \dots, X_I\}, \{X_2, \dots, X_I\}$. However, we also have the conservations of mass and energy

$$\sum_{k=1} F_k = \text{constant},$$

$$\sum_{k=1} k F_k = \text{constant},$$

that leads to the P -semiflow

$$\sum_{k=2} (k-1) F_k = \text{constant}.$$

Therefore, similar to the case of C_{12} , it follows that the system is persistent, and we can use the same Lyapunov function as in the proof of Theorem 2.1 to obtain the desired convergence result. ■

Remark 3.1 *If $I < 3$ then $F_k^* \equiv 0$. If $I = 3$ then $F_2^* \equiv 0$ and $F_1^* = \frac{1}{e^\rho - 1}$, $F_3^* = \frac{1}{e^{3\rho} - 1}$ for some $\rho = \rho(P_0)$.*

4 A reaction network approach for the sum of C_{12}, C_{22}, C_{13}

Let us consider the following equations

$$\dot{F}_{k_1} = \mathcal{C}_{12}[F](k_1) + \mathcal{C}_{22}[F](k_1), \quad (4.1)$$

and

$$\dot{F}_{k_1} = \mathcal{C}_{12}[F](k_1) + \mathcal{C}_{22}[F](k_1) + \mathcal{C}_{13}[F](k_1), \quad (4.2)$$

where $\mathcal{C}_{12}, \mathcal{C}_{22}, \mathcal{C}_{13}$ are the operators defined in (2.7), (3.4), (3.11).

The following theorem then follows by exactly the same argument as in Theorem 3.2

Theorem 4.1 *For any initial condition, the solution*

$$F(t) = (F_k(t))_{k \in \mathbb{I}}$$

of the quantum Boltzmann equation (4.1) or (4.2) converges to an equilibrium state $F^ = (F_k^*)_{k \in \mathbb{I}}$, where $F_k^* = \frac{1}{e^{\rho k} - 1}$ for some constant ρ . Moreover, the solution $F(t)$ of (3.4) converges to F^* exponentially fast in the following sense: there exists positive constants C_1, C_2 such that*

$$\max_{k \in \mathbb{I}} |F_k(t) - F_k^*| < C_1 e^{-C_2 t}.$$

Acknowledgements. G. Craciun was supported by NSF grant DMS-1412643. M.-B Tran was supported by NSF Grant RNMS (Ki-Net) 1107444, ERC Advanced Grant DYCON. M.-B Tran would like to thank Professor Linda Reichl and Professor Robert Dorfman for fruitful discussions on the topic. The research was carried on partially while M.-B. Tran was visiting University of Texas at Austin. He would like to thanks the institution for the hospitality.

References

- [1] Thibaut Allemand. Derivation of a two-fluids model for a Bose gas from a quantum kinetic system. *Kinet. Relat. Models*, 2(2):379–402, 2009.
- [2] Ricardo Alonso, Irene Gamba, and Minh-Binh Tran. The Cauchy problem for the quantum Boltzmann equation for bosons at very low temperature. *Submitted*.
- [3] David F. Anderson. A proof of the global attractor conjecture in the single linkage class case. *SIAM J. Appl. Math.*, 71(4):1487–1508, 2011.
- [4] David F. Anderson, Gheorghe Craciun, and Thomas G. Kurtz. Product-form stationary distributions for deficiency zero chemical reaction networks. *Bull. Math. Biol.*, 72(8):1947–1970, 2010.
- [5] M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell. Observation of Bose-Einstein Condensation in a dilute atomic vapor. *Science*, 269(5221):198–201, 1995.
- [6] M. R. Andrews, C. G. Townsend, H.-J. Miesner, D. S. Durfee, D. M. Kurn, and W. Ketterle. Observation of interference between two Bose condensates. *Science*, 275 (5300):637–641, 1997.
- [7] David Angeli, Patrick De Leenheer, and Eduardo D. Sontag. Persistence results for chemical reaction networks with time-dependent kinetics and no global conservation laws. *SIAM J. Appl. Math.*, 71(1):128–146, 2011.
- [8] David Angeli, Patrick De Leenheer, and Eduardo D. Sontag. Persistence results for chemical reaction networks with time-dependent kinetics and no global conservation laws. *SIAM J. Appl. Math.*, 71(1):128–146, 2011.
- [9] James R. Anglin and Wolfgang Ketterle. Bose-Einstein condensation of atomic gases. *Nature*, 416(6877):211–218, 2002.
- [10] Leif Arkeryd and Anne Nouri. Bose condensates in interaction with excitations: a kinetic model. *Comm. Math. Phys.*, 310(3):765–788, 2012.
- [11] Leif Arkeryd and Anne Nouri. A Milne problem from a Bose condensate with excitations. *Kinet. Relat. Models*, 6(4):671–686, 2013.
- [12] Leif Arkeryd and Anne Nouri. Bose condensates in interaction with excitations: a two-component space-dependent model close to equilibrium. *J. Stat. Phys.*, 160(1):209–238, 2015.
- [13] Volker Bach, Sébastien Breteaux, Thomas Chen, Jürg Fröhlich, and Israel Michael Sigal. The time-dependent Hartree-Fock-Bogoliubov equations for bosons. *arXiv preprint arXiv:1602.05171*, 2016.

- [14] Murad Banaji and Gheorghe Craciun. Graph-theoretic approaches to injectivity and multiple equilibria in systems of interacting elements. *Commun. Math. Sci.*, 7(4):867–900, 2009.
- [15] L. Barbara Goss. Cornell, Ketterle, and Wieman share Nobel Prize for Bose-Einstein Condensates. *Search and Discovery. Physics Today online.*, 2001.
- [16] Gérard Ben Arous, Kay Kirkpatrick, and Benjamin Schlein. A central limit theorem in many-body quantum dynamics. *Comm. Math. Phys.*, 321(2):371–417, 2013.
- [17] Chiara Boccato, Serena Cenatiempo, and Benjamin Schlein. Quantum many-body fluctuations around nonlinear schrödinger dynamics. *arXiv preprint arXiv:1509.03837*, 2015.
- [18] N. M. Bogolyubov. On the theory of superfluidity. *J. Phys. (USSR)*, 11:23–32, 1947.
- [19] L. Boltzmann. Neuer Beweis zweier Satze uber das Warmegleichgewicht unter mehratomigen Gas-molekulen. *Sitzungsberichte der Kaiserlichen Akademie der Wissenschaften in Wien.*, (95):153–164, 1887.
- [20] F. A. Buot. On the relaxation rate spectrum of phonons. *J. Phys. C: Solid State Phys.*, 5(1):5–14, 1972.
- [21] Torsten Carleman. Sur la théorie de l’équation intégrodifférentielle de Boltzmann. *Acta Math.*, 60(1):91–146, 1933.
- [22] Carlo Cercignani. *Theory and application of the Boltzmann equation*. Elsevier, New York, 1975.
- [23] Carlo Cercignani. *The Boltzmann equation and its applications*, volume 67 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1988.
- [24] Carlo Cercignani, Reinhard Illner, and Mario Pulvirenti. *The mathematical theory of dilute gases*, volume 106 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1994.
- [25] Gheorghe Craciun. Toric Differential Inclusions and a proof of the Global Attractor Conjecture. *Available on arXiv:1501.02860*.
- [26] Gheorghe Craciun, Alicia Dickenstein, Anne Shiue, and Bernd Sturmfels. Toric dynamical systems. *J. Symbolic Comput.*, 44(11):1551–1565, 2009.
- [27] Gheorghe Craciun and Martin Feinberg. Multiple equilibria in complex chemical reaction networks. I. The injectivity property. *SIAM J. Appl. Math.*, 65(5):1526–1546, 2005.

- [28] Gheorghe Craciun, Fedor Nazarov, and Casian Pantea. Persistence and permanence of mass-action and power-law dynamical systems. *SIAM J. Appl. Math.*, 73(1):305–329, 2013.
- [29] Matthew Davis. Dynamics of bose-einstein condensation. *PhD Thesis under the supervision of Keith Burnett*, 2001.
- [30] D-A. Deckert, J. Fröhlich, P. Pickl, and A. Pizzo. Dynamics of sound waves in an interacting Bose gas. *Adv. Math.*, 293:275–323, 2016.
- [31] L. Desvillettes and C. Villani. On the trend to global equilibrium in spatially inhomogeneous entropy-dissipating systems: the linear Fokker-Planck equation. *Comm. Pure Appl. Math.*, 54(1):1–42, 2001.
- [32] L. Desvillettes and C. Villani. On the trend to global equilibrium for spatially inhomogeneous kinetic systems: the Boltzmann equation. *Invent. Math.*, 159(2):245–316, 2005.
- [33] Laurent Desvillettes, Klemens Fellner, and Bao Quoc Tang. Trend to equilibrium for reaction-diffusion systems arising from complex balanced chemical reaction networks. *arXiv preprint arXiv:1604.04536*, 2016.
- [34] R. J. DiPerna and P.-L. Lions. On the Cauchy problem for Boltzmann equations: global existence and weak stability. *Ann. of Math. (2)*, 130(2):321–366, 1989.
- [35] D. S. Durfee and W. Ketterle. Experimental studies of bose-einstein condensation. *Optics Express*, 2(8):299–313, 1998.
- [36] László Erdős, Benjamin Schlein, and Horng-Tzer Yau. Derivation of the Gross-Pitaevskii equation for the dynamics of Bose-Einstein condensate. *Ann. of Math. (2)*, 172(1):291–370, 2010.
- [37] M. Escobedo and J. J. L. Velázquez. Finite time blow-up and condensation for the bosonic Nordheim equation. *Invent. Math.*, 200(3):761–847, 2015.
- [38] Miguel Escobedo, Federica Pezzotti, and Manuel Valle. Analytical approach to relaxation dynamics of condensed Bose gases. *Ann. Physics*, 326(4):808–827, 2011.
- [39] Miguel Escobedo and Minh-Binh Tran. Convergence to equilibrium of a linearized quantum Boltzmann equation for bosons at very low temperature. *Kinetic and Related Models*, 8(3):493–531, 2015.
- [40] M. Feinberg. Lectures on chemical reaction networks. *written version of lectures given at the Mathematical Research Center, University of Wisconsin, Madison WI, 1979. Available at <http://www.crnt.osu.edu/LecturesOnReactionNetworks>*.
- [41] Martin Feinberg. Complex balancing in general kinetic systems. *Arch. Rational Mech. Anal.*, 49:187–194, 1972/73.

- [42] Martin Feinberg. The existence and uniqueness of steady states for a class of chemical reaction networks. *Arch. Rational Mech. Anal.*, 132(4):311–370, 1995.
- [43] C. Gardiner and P. Zoller. Quantum kinetic theory. A quantum kinetic master equation for condensation of a weakly interacting Bose gas without a trapping potential. *Phys. Rev. A*, 55:2902, 1997.
- [44] C. Gardiner and P. Zoller. Quantum kinetic theory. III. Quantum kinetic master equation for strongly condensed trapped systems. *Phys. Rev. A*, 58:536, 1998.
- [45] C. Gardiner and P. Zoller. Quantum kinetic theory. V. Quantum kinetic master equation for mutual interaction of condensate and noncondensate. *Phys. Rev. A*, 61:033601, 2000.
- [46] C. Gardiner and P. Zoller. *Cold Atoms: Volume 2 The Quantum World of Ultra-Cold Atoms and Light Book I: Foundations of Quantum Optics*. Imperial College Press, 2014.
- [47] C. Gardiner and P. Zoller. *Cold Atoms: Volume 4 The Quantum World of Ultra-Cold Atoms and Light Book II: The Physics of Quantum-Optical Devices*. Imperial College Press, 2015.
- [48] C. Gardiner, P. Zoller, R. J. Ballagh, and M. J. Davis. Kinetics of Bose-Einstein condensation in a trap. *Phys. Rev. Lett.*, 79:1793, 1997.
- [49] Robert T. Glassey. *The Cauchy problem in kinetic theory*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1996.
- [50] Manoj Gopalkrishnan, Ezra Miller, and Anne Shiu. A geometric approach to the global attractor conjecture. *SIAM J. Appl. Dyn. Syst.*, 13(2):758–797, 2014.
- [51] Nikuni T. Zaremba E. Griffin, A. Bose-condensed gases at finite temperatures. *Cambridge University Press, Cambridge, 2009*.
- [52] M. Grillakis and M. Machedon. Pair excitations and the mean field approximation of interacting bosons, I. *Comm. Math. Phys.*, 324(2):601–636, 2013.
- [53] J. Gunawardena. Chemical reaction network theory for in-silico biologists. *Lecture notes available online at <http://vcp.med.harvard.edu/papers.html>, 2003*.
- [54] E. D Gust and L. E. Reichl. Collision integrals in the kinetic equations of dilute Bose-Einstein condensates. *arXiv:1202.3418*, 2012.
- [55] E. D Gust and L. E. Reichl. Relaxation rates and collision integrals for Bose-Einstein condensates. *Phys. Rev. A*, 170:43–59, 2013.
- [56] F. Horn. Necessary and sufficient conditions for complex balancing in chemical kinetics. *Arch. Rational Mech. Anal.*, 49:172–186, 1972/73.

- [57] F. Horn. The dynamics of open reaction systems. In *Mathematical aspects of chemical and biochemical problems and quantum chemistry (Proc. SIAM-AMS Sympos. Appl. Math., New York, 1974)*, pages 125–137. SIAM–AMS Proceedings, Vol. VIII. Amer. Math. Soc., Providence, R.I., 1974.
- [58] F. Horn and R. Jackson. General mass action kinetics. *Arch. Rational Mech. Anal.*, 47:81–116, 1972.
- [59] M. Imamovic-Tomasovic and A. Griffin. Quasiparticle kinetic equation in a trapped bose gas at low temperatures. *J. Low Temp. Phys.*, 122:617–655, 2001.
- [60] D. Jaksch, C. Gardiner, K. M. Gheri, and P. Zoller. Quantum kinetic theory. IV. Intensity and amplitude fluctuations of a Bose-Einstein condensate at finite temperature including trap loss. *Phys. Rev. A*, 58:1450, 1998.
- [61] D. Jaksch, C. Gardiner, and P. Zoller. Quantum kinetic theory. II. Simulation of the quantum Boltzmann master equation. *Phys. Rev. A*, 56:575, 1997.
- [62] C. Josserand and Y. Pomeau. Nonlinear aspects of the theory of bose-einstein condensates. *Nonlinearity*, 14(5):R25, 2001.
- [63] C. Josserand, Y. Pomeau, and S. Rica. Self-similar singularities in the kinetics of condensation. *Journal of Low Temperature Physics*, 145(1):231–265, 2006.
- [64] W. Ketterle, D. S. Durfee, D. M. Stamper-Kurn, et al. Making, probing and understanding bose-einstein condensates. *arXiv preprint cond-mat/9904034*, 5, 1999.
- [65] T. R. Kirkpatrick and J. R. Dorfman. Transport theory for a weakly interacting condensed Bose gas. *Phys. Rev. A (3)*, 28(4):2576–2579, 1983.
- [66] T. R. Kirkpatrick and J. R. Dorfman. Transport in a dilute but condensed nonideal bose gas: Kinetic equations. *J. Low Temp. Phys.*, 58:301–331, 1985.
- [67] R. Lacaze, P. Lallemand, Y. Pomeau, and S. Rica. Dynamical formation of a Bose-Einstein condensate. *Phys. D*, 152/153:779–786, 2001. Advances in nonlinear mathematics and science.
- [68] M. Lewin, P. T. Nam, S. Serfaty, and J. P. Solovej. Bogoliubov spectrum of interacting Bose gases. *Comm. Pure Appl. Math.*, 68(3):413–471, 2015.
- [69] David Mitrouskas, Sören Petrat, and Peter Pickl. Bogoliubov corrections and trace norm convergence for the hartree dynamics. *arXiv preprint arXiv:1609.06264*, 2016.
- [70] Toan Nguyen and Minh-Binh Tran. Uniform in time lower bound for solutions to a quantum Boltzmann equation of bosons at low temperatures. *submitted*.
- [71] L.W. Nordheim. On the kinetic methods in the new statistics and its applications in the electron theory of conductivity. *Proc. Roy. Soc. London Ser. A*, 119:689–698, 1928.

- [72] R. Peierls. Zur kinetischen theorie der varmeleitung in kristallen. *Annalen der Physik*, 395(8):1055–1101, 1929.
- [73] R. E. Peierls. Quantum theory of solids. In *Theoretical physics in the twentieth century (Pauli memorial volume)*, pages 140–160. Interscience, New York, 1960.
- [74] N. Proukakis, S. Gardiner, M. Davis, and M. Szymanska. *Cold Atoms: Volume 1 Quantum Gases Finite Temperature and Non-Equilibrium Dynamics*. Imperial College Press, 2013.
- [75] L. E. Reichl. *A modern course in statistical physics*. A Wiley-Interscience Publication. John Wiley & Sons, Inc., New York, fourth edition, 2016.
- [76] L. E. Reichl and E. D Gust. Transport theory for a dilute bose-einstein condensate. *J Low Temp Phys*, 88:053603, 2013.
- [77] N. Rougerie, S. Serfaty, and J. Yngvason. Quantum hall states of bosons in rotating anharmonic traps. *Physical Review A*, 87(2):023618, 2013.
- [78] Robert Seiringer. The excitation spectrum for weakly interacting bosons. *Communications in mathematical physics*, 306(2):565–578, 2011.
- [79] D. V. Semikoz and Igor I. Tkachev. Kinetics of bose condensation. *Physical review letters*, 74(16):3093, 1995.
- [80] D. V. Semikoz and Igor I. Tkachev. Condensation of bosons in the kinetic regime. *Physical Review D*, 55(2):489, 1997.
- [81] H. Spohn. Kinetics of the bose-einstein condensation. *Physica D*, 239:627–634, 2010.
- [82] H. Stoof. Coherent versus incoherent dynamics during bose-einstein condensation in atomic gases. *J. Low Temp. Phys.*, 114:11–108, 1999.
- [83] P. Torma and K. Sengstock. *Cold Atoms: Volume 3 Quantum Gas Experiments Exploring Many-Body States*. Imperial College Press, 2014.
- [84] Uhlenbeck G.E. Uehling, E.A. Transport phenomena in einstein-bose and fermi-dirac gases. *Phys. Rev.*, 43:552–561, 1933.
- [85] Cédric Villani. A review of mathematical topics in collisional kinetic theory. In *Handbook of mathematical fluid dynamics, Vol. I*, pages 71–305. North-Holland, Amsterdam, 2002.
- [86] S. M’etens Y. Pomeau, M.A. Brachet and S. Rica. Théorie cinétique d’un gaz de bose dilué avec condensat. *C. R. Acad. Sci. Paris S’er. IIb M’ec. Phys. Astr.*, 327:791–798, 1999.

- [87] Vladimir E. Zakharov and Sergey V. Nazarenko. Dynamics of the Bose-Einstein condensation. *Phys. D*, 201(3-4):203–211, 2005.
- [88] Nikuni T. Griffin A. Zaremba, E. Dynamics of trapped bose gases at finite temperatures. *J. Low Temp. Phys.*, 116:277–345, 1999.